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Results on DG for HR systems: We wish to adopt a discretization method that combines compactness with high-order accuracy. In standard nite-volume methods, higher-order accuracy relies on piecewise-polynomial reconstruction, which requires extended stencils. Discontinuous Galerkin (DG) methods overcome the draw-back of reconstruction by using extra equations for updating the polynomial representation of state variables.

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LOCAL SCALABLE CFD ALGORITHMS BASED ON FIRST-ORDER PDE'S

AFOSR GRANT NR. F49620-03-1-0226

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Abstract
Hyperbolic-Relaxation (HR) systems of partial differential equations (PDE's) bear the promise of describing rarefied flows in the transition regime ($0.001 < Kn < 10$) much more efficiently than pseudo-particle methods like DSMC. In order to arrive at a maximally efficient numerical methodology a Discontinuous-Galerkin (DG) spatial discretization was combined with a Hancock-type temporal integration scheme. A linear HR system of two equations, describing 1-D advection-diffusion in the equilibrium limit, was used as a test-bed for error analysis and numerical experiments. The new method is more efficient than any of the traditional DG and finite-volume methods tested, and remains accurate in the diffusion limit. The method is ready to be extended to nonlinear systems and multiple dimensions. In addition it was demonstrated that spurious inviscid shocks embedded in viscous shock structures, found on the basis of HR systems, can be avoided by modifying the relaxation term.

Objective
The objective of the current research project is to develop and test numerical methods for Hyperbolic-Relaxation (HR) systems of PDE's. These are first-order systems with (usually stiff) source terms that exhibit hyperbolic behavior (wave propagation) for times small compared to the relaxation time τ ("frozen" physics), but over long times exhibit diffusive behavior ("equilibrium" physics). Such systems are useful, for instance, in describing the flow of rarefied gases, whether in the upper atmosphere (re-entry, braking) or in a MEMS device. Numerical methods for HR systems bear the promise of describing these flows much more efficiently than DSMC (particle) methods, for Knudsen numbers as high as 10. The savings could be orders of magnitude in CPU time for current simulations, greatly reducing the turn-around

time for any design cycle.

Crucial to the success of the HR description is the emergence of numerical methods that are uniformly accurate with regard to the parameter $\Delta t/\tau$, where Δt is the time step used in the scheme. These so-called Asymptotic-Preserving (AP) methods would make it possible to compute flows with widely varying local Knudsen number.
For the design and analysis of numerical methods we use an HR system of only two equations, the so-called "generalized hyperbolic heat equation" (GHHE), which in the equilibrium limit reduces to a single advection-diffusion equation. The system is one-dimensional and is taken to be linear when Fourier analysis is in order; it can be made nonlinear for numerical experimentation.

Past year's progress
This performance report covers the final grant period 9/1/2005 - 4/30/2006; it also serves as final report.

Results on DG for HR systems
We wish to adopt a discretization method that combines compactness with high-order accuracy. In standard finite-volume methods, higher-order accuracy relies on piecewise-polynomial reconstruction, which requires extended stencils. Discontinuous Galerkin (DG) methods overcome the draw-back of reconstruction by using extra equations for updating the polynomial representation of state variables. Currently, the most successful DG methods are semi-discretizations combined with TVD Runge-Kutta (RK) ODE solvers, denoted as RKmDG(k) where m is the order of the RK method and k is the degree of the polynomial basis functions.

DG methods were previously shown [1] to be automatically AP provided the advection speed is small compared to the "frozen" wave speed. This guarantee is lost when the advection speed is comparable to the frozen wave speed, due to diffusive numerical errors stemming from approximating the advection operator. In order to arrive at a DG method that remains AP for a finite advection speed, we started from the method of Arora [2], developed earlier in our group. which uses a locally implicit characteristic method to evaluate the cell-interface fluxes with strong coupling to the source terms. To realize the AP property for all practical values of $\Delta t/\tau$, Arora recommends

a minimum of three flux evaluations for computing the flux integral over one time step. Using Huynh's [3] idea of combining a Hancock-type time integrator with DG spatial discretization ("upwind moment scheme"), we were able to cast Arora's idea in a form that uses locally implicit updates inside a cell, and a standard Riemann solver to couple the cells, thus greatly simplifying the method, and making it more attractive to use.

Our HR model system is of the form

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) = \frac{1}{\epsilon}\mathbf{s}(\mathbf{u}), \tag{1}$$

where $\mathbf{u}$ is the vector of conserved variables, $\mathbf{f}$ is the flux of $\mathbf{u}$, $\mathbf{s}$ is the source term, and ϵ is the nondimensional relaxation time. The numerical results we obtained for the DG-Hancock method are based on a 2×2 linear HR system with $\mathbf{u} = [u, v]^T, \mathbf{f} = [v, u]^T$, and $\mathbf{s} = [0, ru - v]^T$ in Eq.(1). This system has "frozen" wave speeds ± 1 when relaxation is weak ($\epsilon \gg 1$); when the relaxation dominates ($\epsilon \ll 1$), it reduces to the advection-diffusion equation $\partial_t u + r\partial_x u \approx \epsilon(1 - r^2)\partial_{xx} u$, with an "equilibrium" wave speed of r. For stability, $|r| \leq 1$.

The solution representation is piecewise linear ($k = 1$); thus, the gradient of each flow variable evolves according to an independent update equation. Details of the method and the numerical experiments are presented in a conference paper by Suzuki and Van Leer [4]. It requires solving a Riemann problem twice at each cell interface but achieves third-order accuracy in time and space. We solve an initial-value problem on a periodic domain with a harmonic initial condition $u_0 = v_0 \equiv \cos(2\pi x),\ x \in [0, 1]$; the other parameters r, ϵ are chosen so that the reduced equation becomes an advection-dominated advection-diffusion equation ($r = 1/2, \epsilon = 10^{-5}$). The new method is compared with a second-order Godunov-type finite-volume method, HR2, and a DG(1) method, both incorporating the IMEX-RK method [5]. At $t = 300$, when the wave has moved 150 times its own length, while its amplitude has been reduced by about 8%, the new method was seen to be the least dissipative and dispersive of all, whereas the RK2HR2 method produces a completely inaccurate solution. A grid-convergence study confirmed that the new method is third-order accurate, as expected from the truncation-error analysis. In contrast, RK2HR2 and RK2DG(1) show second-order convergence in the L_2-norm.

2. Shock representation by HR systems
Resolved shock structures computed on the basis of standard hyperbolic-relaxation systems include, for most Mach numbers, *embedded discontinuities* (inviscid shocks) that are not validated by DSMC calculations [6]. The appearance of such a discontinuity indicates that the chosen relaxation term is inadequate: it lacks information about the nonlinear characteristic fields of the hyperbolic operator. By modifying the relaxation term we have succeeded, for a nonlinear HR model system, in obtaining the correct viscous shock profile. In order to show that a time-marching scheme can find the proper asymptotic steady solution of an HR system, we used a standard second-order upwind-biased finite-volume scheme with a two-stage time-integrator for the modified system

$$u_t + v_x = 0; \tag{2}$$

$$v_t + f^2 u^2 u_x = -\frac{(v - \frac{1}{2}u^2) f^2 u^2}{U^2 \tau}, \tag{3}$$

with $f = 2.0$, $\tau = 0.1$, and boundary conditions

$$u_{\pm\infty} = \pm U, \quad v_{\pm\infty} = U, \quad U = 1. \tag{4}$$

The original relaxation term was $(v - \frac{1}{2}u^2)/\tau$. Figure 1 shows the numerical results plotted on top of the exact profile, for $\Delta x = 0.075$. There is no trace of an inviscid jump, and the agreement appears to be excellent. For comparison, Figure 2 shows the incorrect profile obtained with the original system; it has an infinite derivative at the origin). A grid-refinement study confirms the second-order convergence of the numerical to the exact solution.

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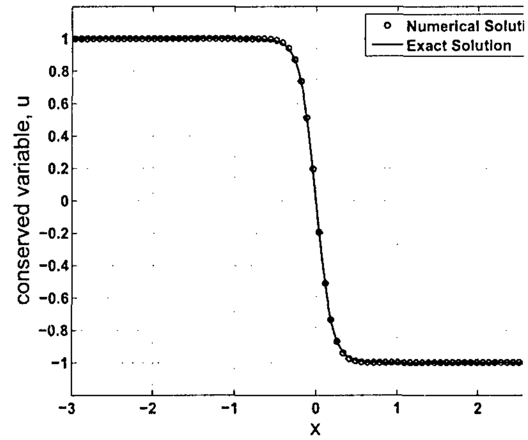

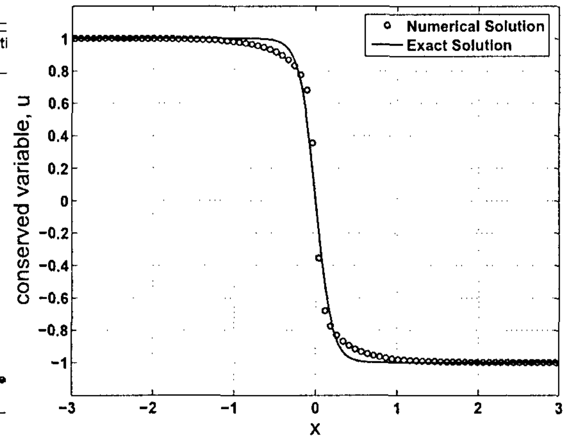

Figure 1: Steady Burgers shock profile (line, exact solution cell averaged) and numerical approximation (symbols) obtained with the modified hyperbolic-relaxation system (3); $\tau = 0.1$, $\Delta x = 0.075$.

Figure 2: Steady Burgers shock profile and numerical approximation obtained with the original hyperbolic-relaxation system; $\tau = 0.1$, $\Delta x = 0.075$. The numerical profile is too steep; its derviative in the origin is infinite.

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Loc Khieu, predoctoral student

Publications

1. Y. Suzuki and B. van Leer, "A discontinuous Galerkin method with Hancock-type time integration for hyperbolic systems with stiff relaxation source terms," presented at the 4th International Conference on Computational Fluid Dynamics, July 10-14, 2006, Gent, Belgium

Honors & Awards Received
In May 2005 Bram van Leer was appointed to Senior Fellow of the University of Michigan. His prior awards include an honorarary doctorate from the Free University of Brussels, two NASA Distinguished Service awards, and the 2003 Computational Mechanics award from the Japan Society of Mechanical Engineers. He was appointed an AIAA Fellow in 1995.

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Transitions
None.

New discoveries
None patentable.